III. Computation and Analysis

DATA SYSTEMS DIVISION

A. Unitary Similarity Transformation of a Hermitian Matrix to a Real Symmetric Tridiagonal Matrix, *R. J. Hanson*

Two known theorems of finite dimensional linear algebra are the following:

Theorem 1. *Every $n \times n$ real symmetric matrix* $\mathbf{A}$, $(\mathbf{A}^T = \mathbf{A})$, *can be written as*

$$\mathbf{A} = \mathbf{V}\mathbf{D}\mathbf{V}^T \tag{1}$$

Here $\mathbf{V}$ *is an* $n \times n$ *real orthonormal matrix,* $(\mathbf{V}^T\mathbf{V} = \mathbf{V}\mathbf{V}^T = \mathbf{I}_n = n \times n$ *identity matrix), and* $\mathbf{D}$ *is a diagonal matrix of real scalars.*

Theorem 2. *Every $n \times n$ hermitian matrix* $\mathbf{A}$,$((\overline{\mathbf{A}})^T = \mathbf{A})$, *can be written as*

$$\mathbf{A} = \mathbf{V}\mathbf{D}(\overline{\mathbf{V}})^T \tag{2}$$

Here $\mathbf{V}$ *is an* $n \times n$ *complex unitary matrix* $((\overline{\mathbf{V}})^T\mathbf{V} = \mathbf{V}(\overline{\mathbf{V}})^T = \mathbf{I}_n)$ *and* $\mathbf{D}$ *is a diagonal matrix of real scalars.* In Eq. (2) the bar over $\mathbf{V}$ denotes complex conjunction.

These theorems have been well known for a long time (Ref. 1). Frequently there are applications where the matrices $\mathbf{V}$ and $\mathbf{D}$ of Eqs. (1) and (2) must be computed numerically.

A great deal of research has been devoted to this numerical problem. This has resulted in one of the most astounding algorithms in all of numerical mathematics. It is usually called the "QR algorithm for symmetric tridiagonal matrices" (Ref. 2). *With this algorithm the construction of the matrices* $\mathbf{V}$ *and* $\mathbf{D}$ *of Eq. (1) can be done with remarkable speed and accuracy in the special case that* $\mathbf{A}$ *is real and tridiagonal, or zero above and below the first super- and sub-diagonal* (Refs. 3 and 4).

The remarks which follow will show how an orthonormal or unitary transformation $\mathbf{W}$ can be explicitly constructed so that

$$\mathbf{A} = \mathbf{W}\mathbf{B}\mathbf{W}^T \tag{3}$$

if $\mathbf{A}$ is symmetric, or

$$\mathbf{A} = \mathbf{W}\mathbf{B}(\overline{\mathbf{W}})^T \tag{4}$$

if $\mathbf{A}$ is hermitian.

The matrix $\mathbf{B}$ of Eq. (3) or (4) is real, symmetric, and tridiagonal. Thus the powerful and elegant QR algorithm

can be used to compute $\mathbb{X}$ and $\mathbb{D}$ of the right side of the equation:

$$\mathbb{B} = \mathbb{X}\mathbb{D}\mathbb{X}^T \tag{5}$$

Here $\mathbb{X}$ is an orthonormal $n \times n$ matrix and $\mathbb{D}$ is a real diagonal matrix of scalars. Finally, $\mathbb{V} = \mathbb{W}\mathbb{X}$. The details regarding the reduction of real symmetric matrices to tridiagonal form have appeared in the literature in detailed algorithmic form (Ref. 5).

To this author's knowledge the details for the reduction of the general hermitian matrix to tridiagonal, real symmetric form have not appeared in the literature.

It should be remarked that there is a naive method for finding the expansion of Eq. (2) using a computational capacity for the case of real symmetric matrices. To see this, write the $n \times n$ hermitian matrix

$$\mathbf{A} = \mathbf{A}_1 + i\mathbf{A}_2, \qquad (i = \sqrt{-1})$$

where the $\mathbf{A}_j$, $(j = 1,2)$, are real.

Then the $2n \times 2n$ symmetric matrix

$$\hat{\mathbf{A}} = \begin{pmatrix} \mathbf{A}_1, & -\mathbf{A}_2 \\ \mathbf{A}_2, & \mathbf{A}_1 \end{pmatrix}$$

has each of the eigenvalues of $\mathbf{A}$ repeated as pairs, and the corresponding $2n$ real eigenvectors $\hat{\mathbf{v}}_j = (\hat{\mathbf{v}}_{1j}^T, \hat{\mathbf{v}}_{2j}^T)^T$ of $\hat{\mathbf{A}}$, where each $\hat{\mathbf{v}}_{\ell j}$, $(\ell = 1,2)$, is a real n vector, are such that $\mathbf{v}_j = \hat{\mathbf{v}}_{1j} + i\hat{\mathbf{v}}_{2j}$ is an eigenvector of $\mathbf{A}$. The matrix $\mathbf{V}$, whose columns are the appropriate members of the $\mathbf{v}_j$, is unitary.

This reformulation of Eq. (2) is *unsatisfactory* for at least three reasons:

(1) About twice as much storage and computer time is used for computing the expression of Eq. (1) for a $2n \times 2n$ real matrix as for the expansion of Eq. (2) for an $n \times n$ hermitian matrix.

(2) Accuracy is unnecessarily lost with twice as many computer operations.

(3) There is a possible programming difficulty in "reshuffling" the eigenvalues and eigenvectors of $\hat{\mathbf{A}}$ to obtain an expansion as in Eq. (2).

For these reasons a subroutine HERMQR has been implemented for the computation of the hermitian eigenproblem. (The subroutine is currently available in the JPL Computation and Analysis Section Subroutine Library.)

To ease the notation which follows we define

$$\mathbf{C}^H = (\bar{\mathbf{C}})^T \tag{6}$$

Thus $\mathbf{C}^H$ denotes the conjugate transpose of any general $m \times n$ complex matrix $\mathbf{C}$.

We next state

Lemma 1. (***Householder Unitary Transformation***). *Let* $\mathbf{x} = [x_1, \cdots, x_n]^T$ *be an arbitrary complex n vector. Let* $k \geq 0$ *be an integer such that* $k + 1 \leq n$.

Define

(1) The integer $\ell = k + 1$

(2) The complex number $(c,s) =$
$$\begin{cases} x_\ell / |\, x_\ell \,|, x_\ell \neq 0, (c^2 + s^2 = 1)^\dagger \\ (1,0), x_\ell = 0 \end{cases}$$

(3) The scalar $t = -(c,s)\,(|\, x_\ell \,|^2 + \cdots + |\, x_n \,|^2)^{1/2}$

(4) The scalars $u_\ell = x_\ell - t, u_j = x_j, (j = \ell + 1, \cdots, n)$

(5) The vector $\mathbf{u} = [0, \cdots, 0, u_\ell, u_{\ell+1}, \cdots, u_n]^T$

(6) The scalar $b = \bar{t}u_\ell$

Then the transformation

$$\mathbf{Q} = \mathbf{I}_n + \mathbf{u}\mathbf{u}^H/b \tag{7}$$

satisfies:

(1) $\mathbf{Q}$ *is unitary, and hermitian* $(\mathbf{Q}\mathbf{Q}^H = \mathbf{Q}^H\mathbf{Q} = \mathbf{Q}^2 = \mathbf{I}_n)$

(2) $\mathbf{Q}\mathbf{x} = [x_1, \cdots, x_k, t, 0, \cdots, 0]^T$

(See Ref. 6.)

We also state

Lemma 2. *Let* $\mathbf{A}$ *be an* $n \times n$ *hermitian matrix with* $n \geq 3$ *and write*

$$\mathbf{A} = \begin{pmatrix} a & \mathbf{x}^H \\ \mathbf{x} & \mathbf{B} \end{pmatrix}$$

where a is a real scalar, $\mathbf{x}$ *is an* $(n-1)$ *complex vector and* $\mathbf{B}$ *is* $(n-1) \times (n-1)$ *and hermitian.*

†SPS 37-55, Vol. III, pp. 28–30.

From Lemma 1, define $\mathbf{Q}$ *so that*

$$\mathbf{Q}[a,\mathbf{x}^T]^T = [a,t,0,\cdots,0]^T$$

where $|t| = ||\mathbf{x}|| =$ *euclidean length of* $\mathbf{x}$.

Then the similarity transformation $\mathbf{A}_1 = \mathbf{QAQ}^H = \mathbf{QAQ}$ *satisfies*:

(1)
$$\mathbf{A}_1 = \begin{pmatrix} a & \bar{t} & 0 & \cdots & 0 \\ t & & & & \\ 0 & & & & \\ \vdots & & \mathbf{B}_1 & & \\ 0 & & & & \end{pmatrix}$$

where $\mathbf{B}_1$ *is hermitian.*

(2) $\mathbf{B}_1$ *is computed from the identity*

$$\mathbf{A}_1 = \mathbf{A} + \mathbf{yu}^H + \mathbf{uy}^H$$

where $\mathbf{y} = (\mathbf{I}_n + \mathbf{uu}^H/2b)\mathbf{Au}/b$.

By successive application of Lemma 2, $n-2$ transformations, $\mathbf{Q}_1, \cdots, \mathbf{Q}_{n-2}$, can be constructed so that

$$\mathbf{Q}_{n-2}\cdots\mathbf{Q}_1\mathbf{AQ}_1\cdots\mathbf{Q}_{n-2} = \mathbf{T}$$

where

$$\mathbf{T} = \begin{pmatrix} a_1 & \bar{b}_1 & & & 0 \\ b_1 & & \ddots & & \\ & \ddots & & \ddots & \bar{b}_{n-1} \\ 0 & & \ddots & b_{n-1} & a_n \end{pmatrix} \qquad (8)$$

is a tridiagonal hermitian matrix.

In conclusion, the following are summarized:

(1) The matrix product $\mathbf{Y} = \mathbf{Q}_1\cdots\mathbf{Q}_{n-2}$ can overwrite the entirety of the working array which holds $\mathbf{A}$ in storage without additional computer storage requirements.

(2) A diagonal unitary transformation, $\mathbf{Z}$, can easily be constructed so that $\mathbf{B} = \mathbf{ZTZ}^H$ is real, tridiagonal and symmetric. The eigenvalues and eigenvectors of $\mathbf{B}$ can be found by the QR algorithm.

(3) The entire computation can be arranged so that (a) only the upper triangular part of $\mathbf{A}$ is used for computing, (b) the eigenvectors for $\mathbf{A}$ overwrite the entirety of the working array which holds $\mathbf{A}$ in storage, and (c) only n additional complex entries are required in the machine.

References

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